

Refine Search

Search Results -

Terms	Documents
3\$1cyano\$12,4,5\$1trifluoro\$1benzoyl chloride	9

Database:

US Pre-Grant Publication Full-Text Database
 US Patents Full-Text Database
 US OCR Full-Text Database
 EPO Abstracts Database
 JPO Abstracts Database
 Derwent World Patents Index
 IBM Technical Disclosure Bulletins

Search:

L5



Refine Search

Recall Text



Clear

Interrupt

Search History

 DATE: Friday, September 02, 2005 [Printable Copy](#) [Create Case](#)

 Set Name Query
 side by side

 Hit Count Set Name
 result set

DB=USPT,USOC,EPAB,JPAB,DWPI,TDBD; PLUR=YES; OP=ADJ

<u>L5</u>	3\$1cyano\$12,4,5\$1trifluoro\$1benzoyl chloride	9	<u>L5</u>
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DB=USPT; PLUR=YES; OP=ADJ

<u>L4</u>	L3 same chlorinat\$7	13	<u>L4</u>
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<u>L3</u>	benzoyl chloride same benzoyl fluoride	71	<u>L3</u>
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<u>L2</u>	L1 and chlorinat\$7	44	<u>L2</u>
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<u>L1</u>	benzoyl chloride and benzoyl fluoride	107	<u>L1</u>
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END OF SEARCH HISTORY

Hit List

[Clear](#)[Generate Collection](#)[Print](#)[Fwd Refs](#)[Bkwd Refs](#)[Generate OACS](#)

Search Results - Record(s) 1 through 9 of 9 returned.

☐ 1. Document ID: US 6706918 B2

--: Invalid display element.

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KWIC	Draw. Des
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☐ 2. Document ID: US 6541675 B2

--: Invalid display element.

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KWIC	Draw. Des
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☐ 3. Document ID: US 6432948 B1

--: Invalid display element.

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KWIC	Draw. Des
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☐ 4. Document ID: US 6323213 B1

--: Invalid display element.

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KWIC	Draw. Des
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☐ 5. Document ID: US 6288081 B1

--: Invalid display element.

Full	Title	Citation	Front	Review	Classification	Date	Reference	Sequences	Attachments	Claims	KWIC	Draw. Des
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☐ 6. Document ID: US 6278013 B1

-: Invalid display element.

Full	Title	Citation	Front	Review	Classification	Date	Reference	Search	Patent	Claims	KMC	Draw. Des
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☐ 7. Document ID: US 6229040 B1

-: Invalid display element.

Full	Title	Citation	Front	Review	Classification	Date	Reference	Search	Patent	Claims	KMC	Draw. Des
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☐ 8. Document ID: US 6133260 A

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Full	Title	Citation	Front	Review	Classification	Date	Reference	Search	Patent	Claims	KMC	Draw. Des
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☐ 9. Document ID: CN 1119324 C, DE 19717231 A1, WO 9847862 A1, AU 9872163 A, EP 977729 A1, CN 1252789 A, HU 200003076 A2, US 6229040 B1, KR 2001005868 A, US 20010023300 A1, JP 2001521534 W, EP 977729 B1, DE 59803342 G, ES 2174431 T3, US 6541675 B2, US 20030092929 A1, HU 222056 B1, CN 1436771 A, IL 131974 A, US 6706918 B2, US 20040167350 A1

-: Invalid display element.

Full	Title	Citation	Front	Review	Classification	Date	Reference	Search	Patent	Claims	KMC	Draw. Des
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Clear

Generate Collection

Print

Fwd Refs

Bkwd Refs

Generate OACS

Terms

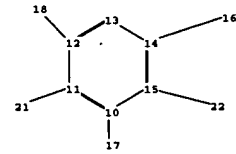
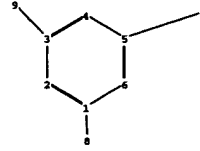
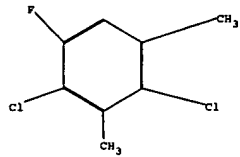
Documents

3\$1cyano\$12,4,5\$1trifluoro\$1benzoyl chloride

9

Display Format: TI

Change Format



⌘
□
■
◆
☞
⌘
■
⌘
◌
📁

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 15:11:21 ON 02 SEP 2005
FILE 'CAPLUS' ENTERED AT 15:11:21 ON 02 SEP 2005
COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	60.02	499.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-7.30	-23.36

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	60.02	499.01

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-7.30	-23.36

FILE 'CASREACT' ENTERED AT 15:11:33 ON 02 SEP 2005
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
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Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 28 Aug 2005 VOL 143 ISS 9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

* CASREACT now has more than 9.2 million reactions *
* *****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\593c.str

L15 STRUCTURE UPLOADED

=> d
L15 HAS NO ANSWERS
L15 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l15
SAMPLE SEARCH INITIATED 15:12:26 FILE 'CASREACT'
SCREENING COMPLETE - 137 REACTIONS TO VERIFY FROM 2 DOCUMENTS

100.0% DONE 137 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 2038 TO 3442

PROJECTED ANSWERS: 0 TO 0

L16 0 SEA SSS SAM L15 (0 REACTIONS)

=> s l15 sss full

FULL SEARCH INITIATED 15:12:41 FILE 'CASREACT'

SCREENING COMPLETE - 212 REACTIONS TO VERIFY FROM 20 DOCUMENTS

100.0% DONE 212 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

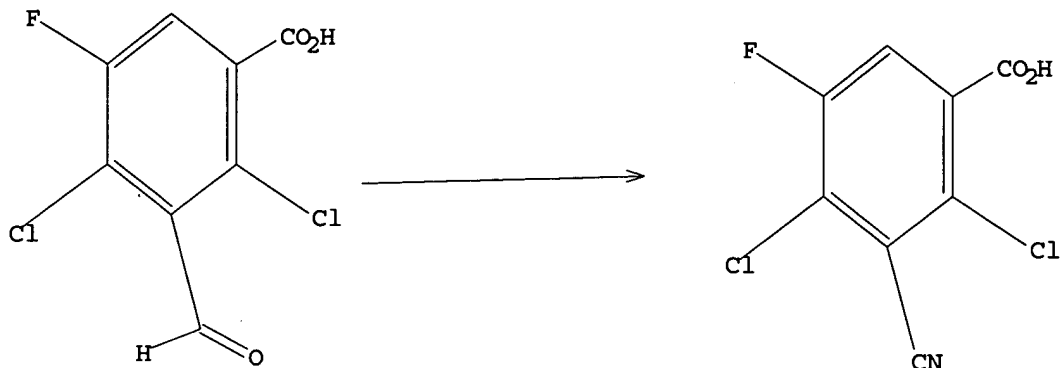
L17 0 SEA SSS FUL L15 (0 REACTIONS)

=>

=>
Uploading C:\Program Files\Stnexp\Queries\593e.str

L23 STRUCTURE UPLOADED

=> d
L23 HAS NO ANSWERS
L23 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l23
SAMPLE SEARCH INITIATED 15:33:03 FILE 'CASREACT'
SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 0 TO 0
PROJECTED ANSWERS: 0 TO 0

L24 0 SEA SSS SAM L23 (0 REACTIONS)

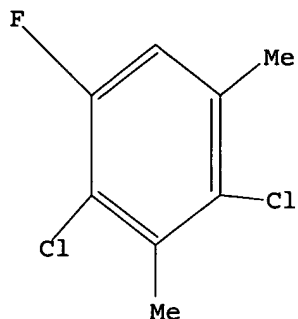
=> s l23 sss full
FULL SEARCH INITIATED 15:33:14 FILE 'CASREACT'
SCREENING COMPLETE - 0 REACTIONS TO VERIFY FROM 0 DOCUMENTS

100.0% DONE 0 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

L25 0 SEA SSS FUL L23 (0 REACTIONS)

=>

=> d
L26 HAS NO ANSWERS
L26 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l26
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:37:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 38 TO ITERATE

100.0% PROCESSED 38 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 391 TO 1129
PROJECTED ANSWERS: 0 TO 0

L27 0 SEA SSS SAM L26

L28 0 L27

=> s l26 full
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:37:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 695 TO ITERATE

100.0% PROCESSED 695 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L29 1 SEA SSS FUL L26

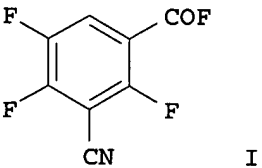
L30 1 L29

=> d ibib abs hitstr

ACCESSION NUMBER: 1998:709043 CAPLUS
DOCUMENT NUMBER: 129:316044
TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and intermediates for its production
INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19717231	A1	19981029	DE 1997-19717231	19970424
CA 2287176	AA	19981029	CA 1998-2287176	19980414
AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
HK 1027555	A1	20040514	HK 2000-106792	20001025
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
US 2004167350	A1	20040826	US 2003-749593	20031231
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
			WO 1998-EP2175	W 19980414
			US 1999-403263	A3 19991015
			US 2001-814132	A1 20010321
			US 2002-227310	A3 20020826

GI



AB 3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II, and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

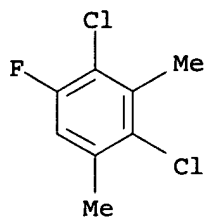
IT 214774-61-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and chlorination of)

RN 214774-61-5 CAPLUS

CN Benzene, 2,4-dichloro-1-fluoro-3,5-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

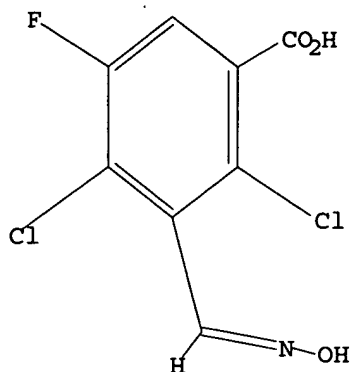
=>

L18 STRUCTURE UPLOADED

=> d

L18 HAS NO ANSWERS

L18 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l18

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 15:22:33 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L19 0 SEA SSS SAM L18

L20 0 L19

=> s l18 sss full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 15:22:44 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

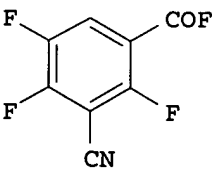
L21 1 SEA SSS FUL L18

=> d ibib abs hitstr

L22 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:709043 CAPLUS
DOCUMENT NUMBER: 129:316044
TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and intermediates for its production
INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter
PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19717231	A1	19981029	DE 1997-19717231	19970424
CA 2287176	AA	19981029	CA 1998-2287176	19980414
AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
HK 1027555	A1	20040514	HK 2000-106792	20001025
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
US 2004167350	A1	20040826	US 2003-749593	20031231
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
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			US 1999-403263	A3 19991015
			US 2001-814132	A1 20010321
			US 2002-227310	A3 20020826

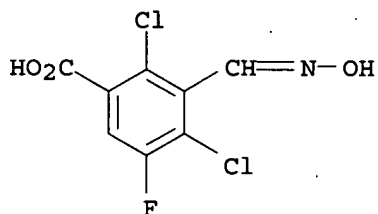
GI



I

AB 3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-

• (trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic
 acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II,
 and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.
 IT 214774-57-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and chlorination-dehydration of)
 RN 214774-57-9 CAPLUS
 CN Benzoic acid, 2,4-dichloro-5-fluoro-3-[(hydroxyimino)methyl]- (9CI) (CA
 INDEX NAME)



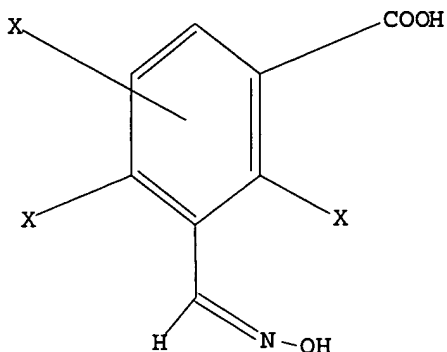
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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>
Uploading C:\Program Files\Stnexp\Queries\593a.str

L2 STRUCTURE UPLOADED

=> d
L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l2
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:52:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 99 TO ITERATE

100.0% PROCESSED 99 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 1384 TO 2576
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L2

L4 0 L3

=> s l2 sss full
REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 14:52:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1932 TO ITERATE

100.0% PROCESSED 1932 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L5 0 SEA SSS FUL L2

L6

0 L5

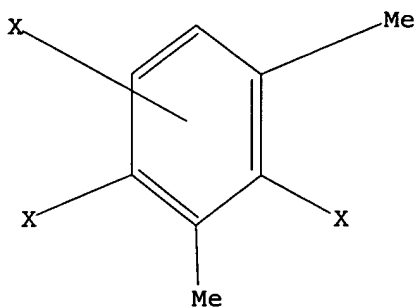
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L7 STRUCTURE UPLOADED

=> d

L7 HAS NO ANSWERS

L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 17

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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SAMPLE SCREEN SEARCH COMPLETED - 6255 TO ITERATE

32.0% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

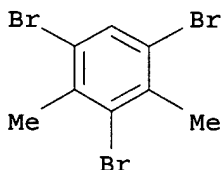
5 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 120359 TO 129841
PROJECTED ANSWERS: 75 TO 549

=> d 1-10 ibib abs hitstr

L14 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

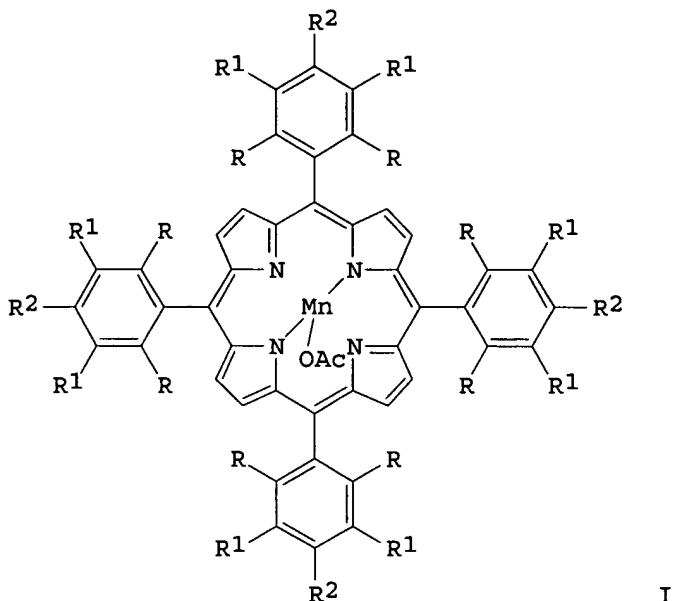
ACCESSION NUMBER: 1991:428577 CAPLUS
DOCUMENT NUMBER: 115:28577
TITLE: Formation constants in carbon-hydrogen hydrogen bonding. 2. Alkynes and polyhalobenzenes with hexamethylphosphoric triamide in cyclohexane solution
AUTHOR(S): Lorand, John P.; Nelson, Jonathan P.; Gilman, R. Dean; Staley, Kathy L.; Chambers, Jeffery R.; Kirk, Harold D.; Moeggenborg, Kevin J.; Farlow, David L.
CORPORATE SOURCE: Dep. Chem., Cent. Michigan Univ., Mt. Pleasant, MI, 48859, USA
SOURCE: Journal of Physical Organic Chemistry (1990), 3(10), 659-69
CODEN: JPOCEE; ISSN: 0894-3230
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Formation consts., K, for hydrogen bonding of weak C-H donors with hexamethylphosphoric triamide were measured in cyclohexane at 35° by PMR, data were analyzed by the Higuchi method. Donors include terminal alkynes and polyfluoro-, polychloro-, and polybromobenzenes. The K values for many of these are too small to measure in CCl4. For RC.tplbond.CH, K decreases in the order R = BrCH2 > C6H5 > C2H5O > tert-Bu. For polyhalobenzenes, K is generally larger for F than Cl or Br, and meta halogens facilitate hydrogen bonding most effectively. Among tetrahalobenzenes, 1,2,3,4-isomers show the least evidence of 2:1 complex formation. Pentachlorobenzene has a smaller K than its 1,2,3,4-tetrachloro analog even after statistical correction; for C6HX5, K decreases in the order F > Cl > Br; the K values for 1,3,5-trihalobenzenes are closely similar; and 1,3,5-tribromo-2,4-dimethylbenzene shows no evidence of hydrogen bonding by PMR. The last three observations suggest that buttressing is important in the C6HX5 structure, at least with Cl and Br. A value of K for benzene was measured, suggesting for the first time that the H atoms of benzene engage in hydrogen bonding. The result compares well with values extrapolated from data for polyfluoro- but not polychlorobenzenes, again probably because of buttressing in the latter.
IT 134636-45-6P, 1,3,5-Tribromo-2,4-dimethylbenzene
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and attempted hydrogen bonding of, to HMPT in cyclohexane)
RN 134636-45-6 CAPLUS
CN Benzene, 1,3,5-tribromo-2,4-dimethyl- (9CI) (CA INDEX NAME)



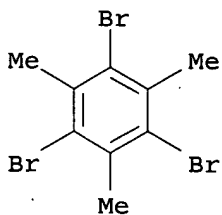
L14 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:473266 CAPLUS
DOCUMENT NUMBER: 109:73266
TITLE: New manganese tetrakis(halogenoaryl)porphyrins featuring sterically hindering electronegative substituents: synthesis of highly stable catalysts in olefin epoxidation
AUTHOR(S): Banfi, Stefano; Montanari, Fernando; Quici, Silvio
CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milano, Milan, 20133, Italy
SOURCE: Journal of Organic Chemistry (1988), 53(12), 2863-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal

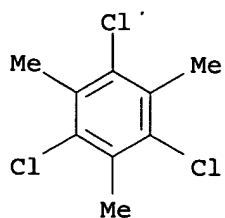
LANGUAGE: English
 OTHER SOURCE(S): CASREACT 109:73266
 GI



AB The complexes I (R = R2 = Cl, Br, R1 = Me; R = R2 = H, R1 = Cl) were prepared from halomesitylenes via condensation of halobenzaldehydes with pyrrole and complexation with Mn(OAc)2. I (R = Cl, R1 = R2 = H; R = R2 = Cl, Br, R1 = Me) are highly stable and efficient catalysts for the epoxidn. of cyclooctene and 1-dodecene with NaOCl at pH 9.5 and 0° under two-phase conditions, in the presence of N-hexylimidazole as axial ligand. The chemical stability dramatically decreases in I (R-R2 = H, F; R = R2 = Me, R1 = H; R = R2 = H, R1 = Cl).
 IT 608-72-0, 2,4,6-Tribromomesitylene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conversion to dimethyltribromobenzyl alc.)
 RN 608-72-0 CAPLUS
 CN Benzene, 1,3,5-tribromo-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



IT 5324-68-5, 2,4,6-Trichloromesitylene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conversion to dimethyltrichlorobenzyl alc.)
 RN 5324-68-5 CAPLUS
 CN Benzene, 1,3,5-trichloro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)

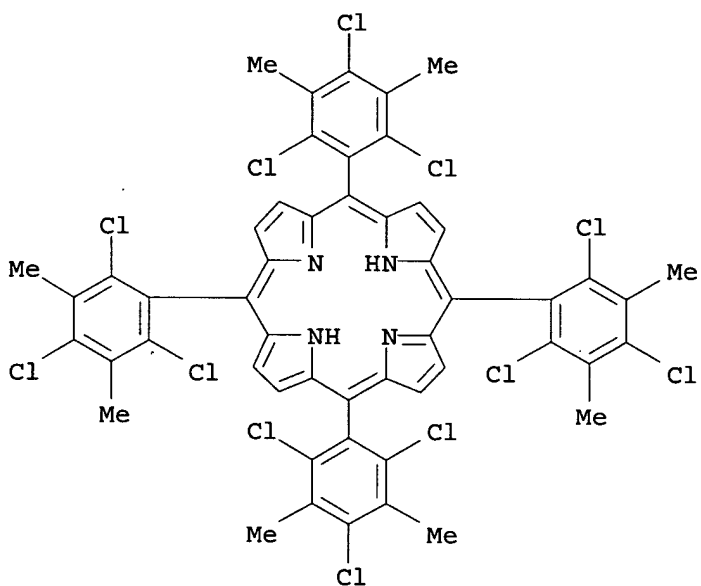


IT 114634-36-5P 114634-37-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with manganese)

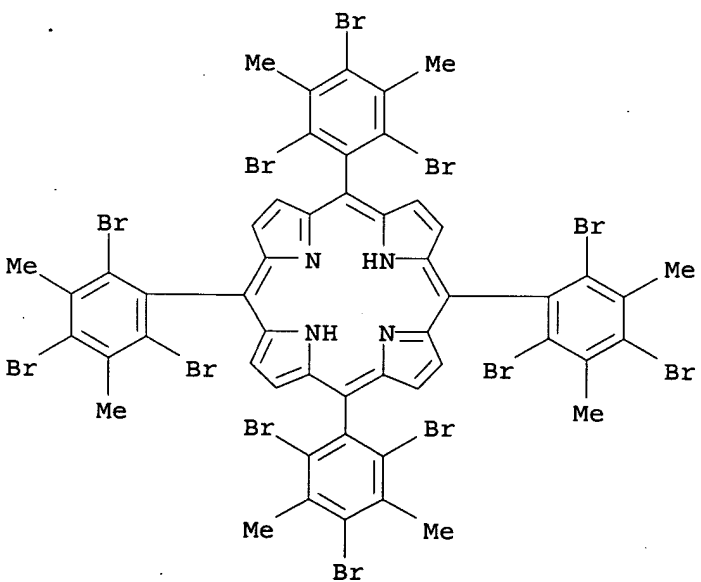
RN 114634-36-5 CAPLUS

CN 21H,23H-Porphine, 5,10,15,20-tetrakis(2,4,6-trichloro-3,5-dimethylphenyl) -
(9CI) (CA INDEX NAME)

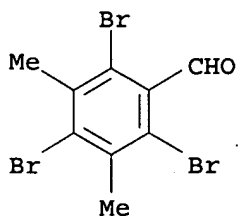


RN 114634-37-6 CAPLUS

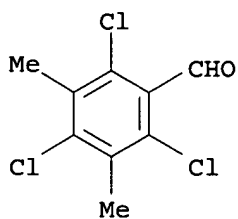
CN 21H,23H-Porphine, 5,10,15,20-tetrakis(2,4,6-tribromo-3,5-dimethylphenyl) -
(9CI) (CA INDEX NAME)



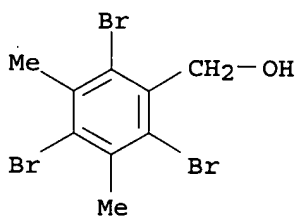
IT 114634-34-3P 114634-35-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and coupling of, with pyrrole)
 RN 114634-34-3 CAPLUS
 CN Benzaldehyde, 2,4,6-tribromo-3,5-dimethyl- (9CI) (CA INDEX NAME)



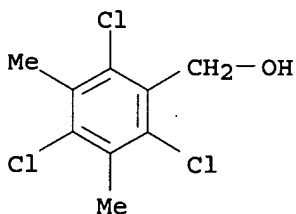
RN 114634-35-4 CAPLUS
 CN Benzaldehyde, 2,4,6-trichloro-3,5-dimethyl- (9CI) (CA INDEX NAME)



IT 114634-32-1P 114634-33-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and oxidation of)
 RN 114634-32-1 CAPLUS
 CN Benzenemethanol, 2,4,6-tribromo-3,5-dimethyl- (9CI) (CA INDEX NAME)

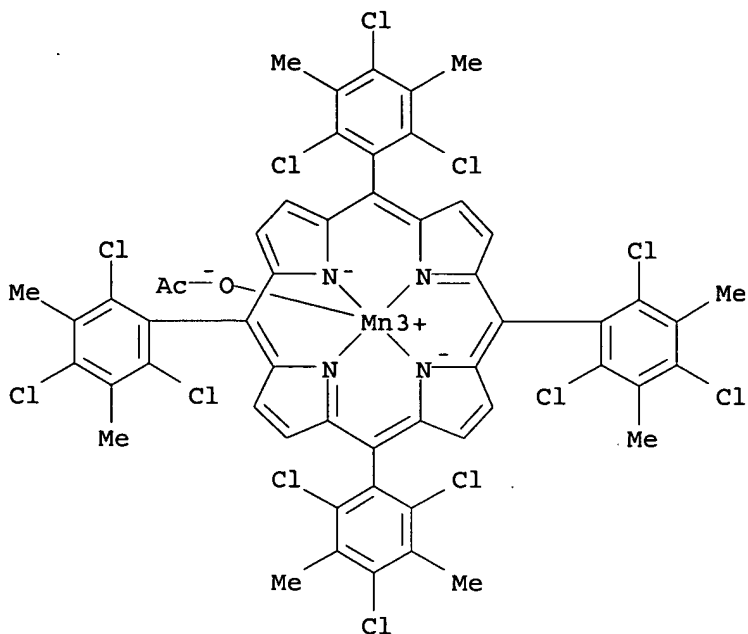


RN 114634-33-2 CAPLUS
 CN Benzenemethanol, 2,4,6-trichloro-3,5-dimethyl- (9CI) (CA INDEX NAME)

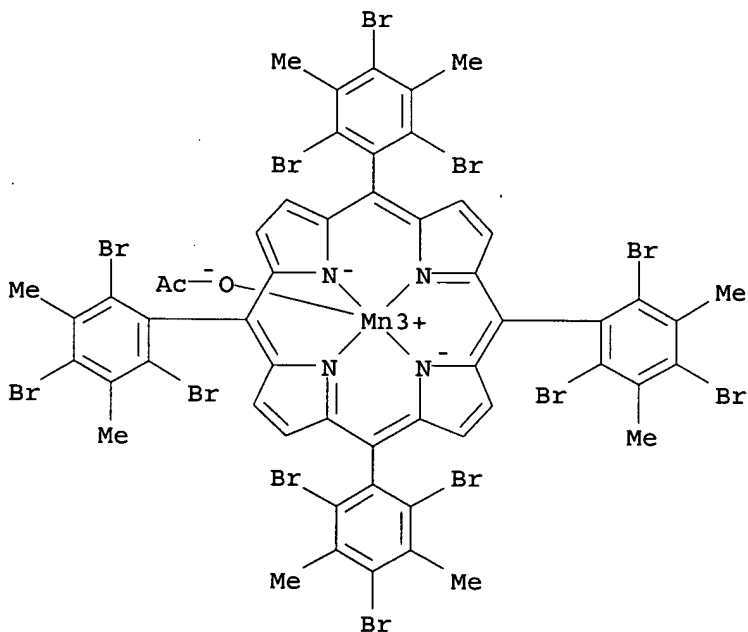


IT 114651-81-9P 114651-82-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as epoxidn. catalyst, stability of)
 RN 114651-81-9 CAPLUS
 CN Manganese, (acetato-O) [5,10,15,20-tetrakis(2,4,6-trichloro-3,5-

dimethylphenyl)-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9Cl)
(CA INDEX NAME)



RN 114651-82-0 CAPLUS
CN Manganese, (acetato-O) [5,10,15,20-tetrakis(2,4,6-tribromo-3,5-dimethylphenyl)-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9Cl)
(CA INDEX NAME)



L14 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:422689 CAPLUS

DOCUMENT NUMBER: 87:22689

TITLE: Permercured arenes. Part II. Synthesis of perbromobenzoic acids and perbromobenzenes from aromatic carboxylic acids by permercuration and bromodemercuration

AUTHOR(S): Deacon, Glen B.; Farquharson, Graeme J.

CORPORATE SOURCE: Chem. Dep., Monash Univ., Clayton, Australia
 SOURCE: Australian Journal of Chemistry (1977),
 30(2), 293-303
 CODEN: AJCHAS; ISSN: 0004-9425

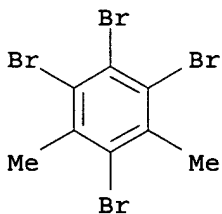
DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Mercuration of RC6H4CO2H (R = 2-Me, -Cl, -F, and -Br, 3-Me, -F, -Cl, -Br, -CF3, -NO2, and -OMe, and 4-Me, -F, -Cl, -Br, -CF3, and -NO2) and 2,6-R2C6H3CO2H (R = Me, Cl, Br) with (CF3CO2)2Hg and subsequent bromodemercuration gave the resp. RC6Br4CO2H and 2,6-R2C6Br3CO2H, which were accompanied by C6Br5R and 1,3-R2C6Br4.

IT 39568-70-2P
 RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 39568-70-2 CAPLUS

CN Benzene, 1,2,3,5-tetrabromo-4,6-dimethyl- (9CI) (CA INDEX NAME)



L14 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:179885 CAPLUS

DOCUMENT NUMBER: 84:179885

TITLE: Quality of phthalic acids improved by haloacetic acid

INVENTOR(S): Kuhlmann, George E.

PATENT ASSIGNEE(S): Standard Oil Co., USA

SOURCE: U.S., 6 pp.
 CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3947494	A	19760330	US 1972-316857	19721220 <--

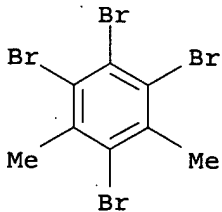
PRIORITY APPLN. INFO.: US 1972-316857 A 19721220

AB Phthalic acids of improved quality were obtained by direct oxidation of xylenes (e.g., o- and p-xylene, m- and p-Me2C6Br4, p-Me2C6Cl4) with O in an oxidation zone with small amts. of haloacetic acid, e.g., XCH2CO2H (X = Cl, Br, F) or F3CCO2H, present in HOAc solution of one or more heavy metal oxidation catalysts and Br-releasing Br-containing compound BrCH2CO2H was the most effective acid tested.

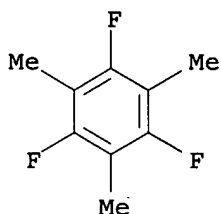
IT 39568-70-2
 RL: RCT (Reactant); RACT (Reactant or reagent) (oxidation of, effect of haloacetic acids on quality of phthalic acids from)

RN 39568-70-2 CAPLUS

CN Benzene, 1,2,3,5-tetrabromo-4,6-dimethyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1972:447779 CAPLUS
 DOCUMENT NUMBER: 77:47779
 TITLE: Stable carbocations. CXXXIX. Nitro- and chlorohexamethylbenzeneium ions and 1-nitro- and 1-chloro-2,4,6-trifluoromesitylenium ions
 AUTHOR(S): Olah, George A.; Lin, Henry C.; Mo, Y. K.
 CORPORATE SOURCE: Dep. Chem., Case West. Reserve Univ., Cleveland, OH, USA
 SOURCE: Journal of the American Chemical Society (1972), 94(10), 3667-9
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Hexamethylbenzeniums (I, X = NO₂, Cl) and 2,4,6-trifluoromesityleniums (II, X = NO₂, Cl) were obtained by treating Me₆C₆ or 1,3,5,2,4,6-F₃Me₃C₆ with NO₂+BF₄-FSO₃H-SO₂ and SbF₅-FSO₃H-Cl₂-SO₂ClF solution at low temperature. The structure of the ions were confirmed by PMR and F NMR. The PMR of I (R = NO₂) is temperature dependent indicating the degenerate migration or exchange process of the nitro group (NO₂⁺). The energy of activation of the process was 16.8 ± 1.5 kcal/mole.
 IT 363-64-4
 RL: PRP (Properties)
 (benzenium ion formation from)
 RN 363-64-4 CAPLUS
 CN Benzene, 1,3,5-trifluoro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1963:441438 CAPLUS
 DOCUMENT NUMBER: 59:41438
 ORIGINAL REFERENCE NO.: 59:7428d-h,7429a-c
 TITLE: Perchloryl aromatic compounds
 INVENTOR(S): Inman, Charles E.; Oesterling, Robert E.; Tyezkowski, Edward A.
 PATENT ASSIGNEE(S): Pennsalt Chemicals Corp.
 SOURCE: 12 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3076853		19630205	US	19620621 <--

AB The title compds. ArClO₃ were prepared by treating the appropriate aromatic compound with ClO₃F in the presence of a Freidel-Crafts catalyst. AlCl₃ was the preferred catalyst. An excess of the aromatic compound or an inert solvent may be used. Thus, AlCl₃ 133 was suspended with agitation in benzene 2600 parts in a cooling bath. ClO₃F gas 100 patts was slowly passed into the mixture and the temperature maintained at 40°. Gaseous HCl was evolved. After HCl evolution had ceased, the reaction mass was added to twice its volume of H₂O, and steam-distilled. The benzene layer was evaporated and distilled in vacuo to give perchlorylbenzene 62 parts, b. 232°, f.p. -3°, n_D²⁰ 1.5236, d₃₀ 1.185. Similarly prepared were the following substituted perchlorylbenzenes [substituent(s) given]: 2,4-dimethyl; 2,5-dimethyl (b₂ 78°, m. 27-8°); 4-fluoro

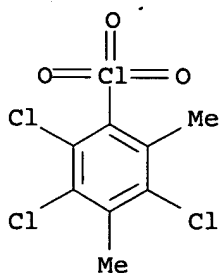
(b0,25 53°,n2D0 1.5051); 2,5dibromo; 2,5-dimethyl; 2,5-difluoro; 3,4-dimethyl; 4-hydroxy; 3,4-dibromo; 2,4-dimethyl; 2,5-dimethyl-4-chloro; 3,4,5-trichloro; 2,5-dichloro-3-fluoro; 2,4,6-trimethyl; 2,3,5,6-tetramethyl; 2-chloro-5-fluoro. A solution of perchlorylbenzene 20 in concentrated H2SO480 was treated with a mixture of concentrated H2SO425 and concentrated HNO3 14 parts at 20-300 for 1 hr. The mixture was poured over ice and a yellow solid 22 parts was filtered from the mixture Recrystn. from benzene-petr. ether gave yellow 3-nitroperchlorylbenzene, m. 49-50°, reduced with SnCl2 in alc. HCl to 3-aminoperchlorylbenzene, m. 32°. The following substituted perchlorylbenzenes were prepared by known methods [substituent(s) given]: B-NH2.HCl; 3-acetamido (m. 136 70); 4-Cl; 4-Me; 3,4-dichloro; 3-amino-4-methyl; 3-amino-4-methyl-6-nitro; 2,3,5-trichloro-4-fluoro; 2,3,5,6-tetrachloro-4-hydroxy-; 3-HO3S; 2-MeO; 2-Cl; 2-chloro-5-nitro; 4-MeS; 3-(4-nitrophenyl); 4nitro-3-(4-nitrophenyl); 2-chloro-5-amino; 2-chloro-3-nitro-5-amino; 2-Me; 3,5,6-trichloro-2-methyl; 3,4,5-trichloro-2-methyl; 2,3,4,5,6-pentachloro; 2,5-dimethyl-3-cyano; 3,4-dichloro-2,5difluoro; 3,6-dichloro-2,5-difluoro; 3,4-dichloro-5-methoxy; 3,4dichloro-5-phenyl; 3,4-dibromo-2,5-dichloro; 2,4-bis(chloromethyl); 2,4,5-trimethyl-3-nitro; 3,4,5-trichloro-2-iodo; 2,4,5,6-tetrachloro-3-fluoro; 3-iodo-2,4,6-trimethyl; 4-amino-2,3,5,6tetramethyl; 3-acetamido-2-nitro; 2,5-diamino-3-chloro; 3(3-perchlorylphenyl); 4-chloromethyl. Also prepared were azobis(3-perchlorylbenzene), azoxybis(3-perchlorylbenzene), and hydrazobis(3-perchlorylbenzene). 3-Aminoperchlorylbenzene-HCl 1 part was dissolved in 20% HCl and diazotized with NaNO2 solution at 0-5° to form a solution of the diazonium salt. Yellow crystals of 3,3'-diperchloryldiazoaminobenzene were removed by filtration. To the filtrate was added β-naphthol 1 part dissolved in dilute NaOH to give dark orange 3-(β-hydroxynaphthylazo)perchlorylbenzene, m. 200-1°. A mixture of 0.0233 mole 4-fluoroperchlorylbenzene and 0.221 mole NaOMe in 200 ml. MeOH was refluxed for 90 min., the cooled mixture diluted with H2O, and extracted with Et25 to give 4-methoxyperchlorylbenzene, n2D0 1.5307. 4-Phenylthioperchlorylbenzene, n2D6 1.5778, was similarly prepared from 4-finorperchlorylbenzene and thiophenol in the presence of Na-OMe. 4-Chloroperchlorylbenzene was also prepared by chlorination of perchlorylbenzene at 10-16° in the presence of 1% anhydrous FeCl3. Other nuclear chlorinated compds. were similarly prepared by continuing chlorination below 280° to substitution tip to 5 Cl atoms. Bromo- and iodoperchlorylbenzene compds. were similarly prepared using the appropriate halide catalyst (FeBr3, iodine, or Fe). Alkylhaloperchloryl aryl compds. were prepared by halogenating the alkylperchloryl aryl compound. Thus, 2,4-dimethyl-perchlorylbenzene was progressively chlorinated, first at 5-10° and then by gradually raising the temperature to 60°, with gaseous Cl in the presence of FeCl3 and in a suitable solvent (ClCH2CCL3, CCL14, PhNO2, Et2O, EtOH, CHCl3, or glacial HO3c) to give 3-chloro-, 3,5-dichloro-, and 3,5,6-trichloro-2,4-dimethylperchlorylbenzene. Chlorination of 2,4-dimethylperchlorylbenzene was carried out in a glass tower packed with glass rings and illuminated with Hg lamps spaced 4 ft. apart. The 2,4-dimethyl-perchlorylbenzene was heated to 65-75° and red into the top of the tower at a uniform rate. Dry Cl gas was passed up the tower. The temperature of the tower was kept just below the reflux point and 2,4-chloromethylperchlorylbenzene was recovered as product. Highly alkylated and hydroxy-containing derivs. of perchlorylbenzene were chloromethylated by treating the perchloryl aryl compound with HCHO and HCl below 280° in the presence of H2SO4, ZnCl2, Al, or Sn as catalysts. Perchlorylbenzene and its homologs were sulfonated by heating a mixture of the perchloryl aryl compound and concentrated H2SO4 below 280°. The title compds. were useful as explosives. 3-(β-Hydroxynaphthylazo)perchlorylbenzene was useful as a dye for wool.

IT 90048-78-5, m-Xylene, 2,4,5-trichloro-6-perchloryl-

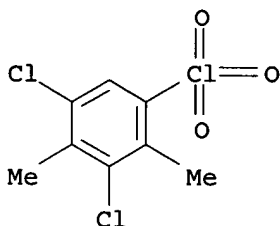
90151-28-3, m-Xylene, 2,4-dichloro-6-perchloryl-
(preparation of)

RN 90048-78-5 CAPLUS

CN m-Xylene, 2,4,5-trichloro-6-perchloryl- (7CI) (CA INDEX NAME)



RN 90151-28-3 CAPLUS
 CN m-Xylene, 2,4-dichloro-6-perchloryl- (7CI) (CA INDEX NAME)



L14 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

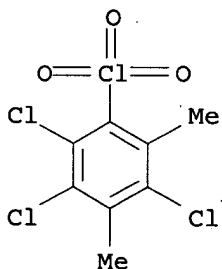
ACCESSION NUMBER: 1963:81229 CAPLUS
 DOCUMENT NUMBER: 58:81229
 ORIGINAL REFERENCE NO.: 58:13841b-h
 TITLE: Perchloryl aromatic compounds
 INVENTOR(S): Inman, Charles E.; Oesterling, Robert E.; Tyezkowski, Edward A.
 PATENT ASSIGNEE(S): Pennsalt Chemicals Corp.
 SOURCE: 12 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3070609		19621225	US	19620621 <--

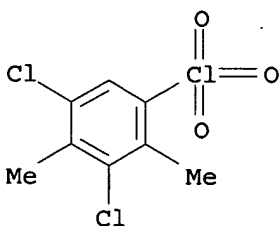
AB The F atom of FClO3 (I) (perchloryl fluoride, b. -47.5°), was replaced with a substituted or unsubstituted aryl radical, by using a new organic unit process, perchlorylation (similarly to nitration, sulfonation, etc.), to form perchloryl aromatic compds. These can be further treated (sulfonated, halogenated, etc.). The new compds. possess explosive properties; they are useful as explosive charges for blasting and for the manufacture of explosive devices, also as high energy fuels, as intermediates in the preparation of compds. useful in pharmaceutical and dye application, as additives for fuels in internal combustion engines, particularly as cetane improvers in diesel fuels. To prepare these compds., I in gaseous form and the aromatic compound (preferably C6H6, or substituted C6H6 as PhMe, PhEt, xylenes, mono-, di-, and trihalobenzenes; and chlorotoluenes) are brought together in stoichiometric proportions in the presence of Friedel-Crafts catalysts, as AtCl3, about mole per mole, in a nonalk., nonaq. system at 0-80° (preferably 0-15° for most of the reactions). Preferably, the catalyst is added to the aromatic compound, with the latter being used alone in excess or dissolved in a nonaq., inert solvent or diluent, and I is then passed into the mixture with agitation. The perchlorylated aromatic compds. can be treated under mildly alkaline, neutral, or acid conditions, below 280° around which temperature the ClO3 group is unstable and the compds. decompose explosively. The ClO3 group is replaced by HO group upon treatment with inorg. or organic base under strongly alkaline conditions. Thus, 133 parts AlCl3 was suspended with agitation in 2600 parts C6H6 in a vessel in a cooling bath. I gas was passed slowly into the C6H6-AlCl3 mixture which was maintained at 40°. HCl gas was evolved from the reaction mass. Addition of I was

stopped when 100 parts had been added and HCl evolution ceased. The reaction mass was added to twice its volume of water. The mass was then steam-distilled. The C₆H₆ layer thus recovered was evaporated, and the PhClO₃ contained therein, 70 parts, was recovered as a pale yellow oil. Distillation in vacuo gave 62 parts PhClO₃, b. 282° f.p. -3° n₂₀D 1.5236, d₃₀ 1.186. Similarly, from m-C₆H₄(CH₃)₂ (with AlCl₃ and I), 2,4-Me₂C₆H₃ClO₃ was obtained, b. 78°. From PhF (with AlCl₃ and I), 4-FC₆H₄ClO₂ was obtained, b. 0.25 53°, n₂₀D 1.5051. From 3-O₂NC₆H₄ClO₃ (with EtOH, concentrated HCl, SnCl₂), 3-H₂NC₆H₄ClO₃ was obtained, m. 32°. From PhClO₃ (with concentrated H₂SO₄, concentrated HNO₃), 3-O₂-NC₆H₄ClO₃ was obtained, m. 49-50°. O₂NC₆H₄Ph (with I and AlCl₃) gave perchlorylnitrobiphenyl. From PhOH (with I and AlCl₃), 4-HOC₆H₄ClO₃ was obtained. From 3-H₂NC₆H₄ClO₃ (with anhydrous ether, anhydrous HCl), the HCl salt was obtained, decomposed. From 3-H₂NC₄H₄ClO₃ (with Ac₂O-AcOH), 3-AcNH-C₆H₄ClO₃ was obtained, m. 136-7° (EtOH). PhClO₃ at atmospheric pressure and 285° detonated vigorously; in liquid and in solid form it exploded when it was subjected to impact on a detonating block. m-O₂-NC₆H₄ClO₃, subjected to impact on a detonating block, exploded, p-O₂NC₆H₄ClO₃ was exploded upon detonation of blasting caps by means of an elec. detonator. 3-H₂NC₆H₄ClO₃.HCl (with 20% HCl, diazotized with NaNO₂ solution) gave 3-O₃ClC₆H₄N: -N NHC₆H₄ClO₃-3, which with β-naphthol in dilute NaOH gave a dye, 3-(β-HOC₁₀H₆N:N)C₆H₄ClO₃, dark orange crystals, m. 200-1°, λ 464 mμ. Wool cloth was dyed with 3-(β-HOC₁₀H₆N:N)C₆H₄-ClO₃ to a deep orange color, which withstood prolonged exposure in the sunlight without appreciable loss of color. 4-FC₆H₄ClO₃ with MeONa-MeOH gave 4-MeOC₆H₄ClO₃, n₂₈D 1.5307. 4-F-C₆H₄ClO₃ with HSPH-MeONa gave 4-PhSC₆H₄ClO₃, n₂₆D 1.5778. From PhClO₃ (with FeCl₃ and gaseous Cl), 4-ClC₆H₄ClO₃, was obtained, all oily liquid.

IT 90048-78-5, m-Xylene, 2,4,5-trichloro-6-perchloryl-
 90151-28-3, m-Xylene, 2,4-dichloro-6-perchloryl-
 (preparation of)
 RN 90048-78-5 CAPLUS
 CN m-Xylene, 2,4,5-trichloro-6-perchloryl- (7CI) (CA INDEX NAME)



RN 90151-28-3 CAPLUS
 CN m-Xylene, 2,4-dichloro-6-perchloryl- (7CI) (CA INDEX NAME)



L14 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

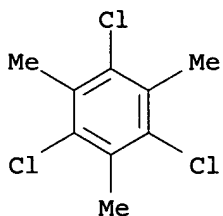
ACCESSION NUMBER: 1955:45417 CAPLUS

DOCUMENT NUMBER: 49:45417

ORIGINAL REFERENCE NO.: 49:8700e-f

TITLE: Absorption spectra in relation to the chemical reactivity of some haloaromatic compounds

AUTHOR(S): Smith, F.; Turton, Lilian M.
 CORPORATE SOURCE: Univ. Birmingham, UK
 SOURCE: Journal of the Chemical Society, Abstracts (1955) 1350-4
 CODEN: JCSAAZ; ISSN: 0590-9791
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB cf. J. Appl. Chemical 4, 325(1954). The ultraviolet-light-absorption spectra of a number of Cl- and F-aromatic compds. are described, and some correlation of the results with the degree of halogenation of the substances and their reactivity is attempted. The spectrophotometric measurements were carried out as previously described (cf. C.A. 45, 8352d).
 IT 5324-68-5, Mesitylene, 2,4,6-trichloro- (spectrum of)
 RN 5324-68-5 CAPLUS
 CN Benzene, 1,3,5-trichloro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)

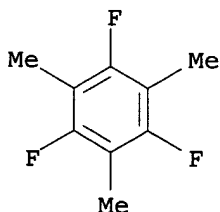


L14 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1953:11438 CAPLUS
 DOCUMENT NUMBER: 47:11438
 ORIGINAL REFERENCE NO.: 47:2036i,2037a-e
 TITLE: Electron distribution in molecules. I. F19 nuclear magnetic shielding and substituent effects in some benzene derivatives
 AUTHOR(S): Gutowsky, H. S.; McCall, D. W.; McGarvey, B. R.; Meyer, L. H.
 CORPORATE SOURCE: Univ. of Illinois, Urbana
 SOURCE: Journal of the American Chemical Society (1952), 74, 4809-17
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 AB The effect of substituents on the electron distribution in benzene produces changes in the nuclear magnetic shielding of F atoms in the mol. A comparison of the F19 nuclear magnetic shielding in PhF with that in a substituted PhF was used in defining a δ -parameter (C.A. 46, 5433b). A radiofrequency spectroscope with slow sweep modulation was used to measure mol. differences in nuclear magnetic shielding. Exptl. δ -values were determined for the following monosubstituted PhF derivs.: o-, m-, and p-NO₂, -CN, -CO₂H, -I, -Br, -Cl, -F, -Me, -NHAc, -OH, -OEt, -NH₂; o- and p-OMe; p-SO₂Cl, -CCl₃, -Ph, -OC₆H₄F, -NHPh, -NMe₂; o-CH:CHCO₂H; m-CF₃, -CH(OH)Me, -OC₆H₄F. A linear correlation was observed between Hammett's substituent constant σ and measured δ values. A least-squares solution for meta derivs. gives $\sigma_m = 1.69\delta_m$ and for para derivs., $\sigma_p = 0.560\delta_p + 0.271$. Systematic differences in the correlation were observed and attributed to the dependence of the δ -values on the nature of the electronic interactions of the substituent. Thereby, a detailed analysis of the δ - and σ -values for particular substituents permits evaluation of the nature of their electronic effects. Consideration of o-substituents suggests that an interaction contributes to the δ_o -values in some cases in addition to the usual inductive and electromeric effects at the m- and p-positions. The potential uses and limitations of δ_o -values in evaluating o-effects and entropies of reaction are discussed. A determination of the extent to which substituent effects are additive was made by measuring δ -values for the

following polysubstituted PhF compds. (observed δ at the 1-position): 3-NO₂, 4-NH₂; 2-NO₂, 4-NH₂; 3, 5-, 2, 4-, 3, 4-, and 2, 5-di-fluoro; 3-F, 5-1; 2, 4-dinitro; 2-NH₂, 4-F; 3-NH₂, 4-F; 2-NH₂, 5-F; 3-F, 4-NH₂; 2-NO₂, 4-F; 3-NO₂, 4-F; 2-NO₂, 5-F; 3-F, 4-NO₂; 2-Cl, 4-F; 3-Cl, 4-F; 2-Cl, 5-F; 3-F, 4-Cl; 2-Br, 4-F; 3-Br, 4-F; 2-I, 4-F; 3-I, 4-F; 2-I, 5-F; 3-F, 4-I; 2-CF₃, 4-F; 3-CF₃, 4-F; 2,4,6-trimethyl; 2,5-dichloro-4-F; 2, 5-dibromo-4-F; 2,4,5-trifluoro; 2, Br-4,5-difluoro; 2,4-difluoro-5-Br; 2,5-difluoro-4-Br; 2,5-difluoro-3-CF₃; 2,4-difluoro-6-CF₃; 3,4-difluoro-5-CF₃; 2,4,6-trimethyl-3-F; 2,4,6-trimethyl-3,5-difluoro. The electronic effects of substituents are usually additive, but there is significant nonadditivity between substituents in about 1/3 of the compds. studied, demonstrating interaction between substituents. A δ' parameter, analogous to δ , is defined in terms of the change produced by a substituent in the ring on the F19 nuclear magnetic shielding in benzotrifluorides. The δ' -values were determined for the following substituted benzotrifluorides: o-, m-, and p-Cl, -CF₃; o- and m-NH₂; m-F, -Br, -NO₂. The δ' -values are about 1/10 of the δ -values for the same substituents; this indicates the extent of attenuation of the substituent effects in the side chain.

IT 363-64-4, Mesitylene, 2,4,6-trifluoro-
(fluorine nuclear magnetic shielding in)
RN 363-64-4 CAPLUS
CN Benzene, 1,3,5-trifluoro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



L14 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1947:8981 CAPLUS
DOCUMENT NUMBER: 41:8981
ORIGINAL REFERENCE NO.: 41:1870a-i,1871a
TITLE: Vulcanization of GR-S with halogen compounds
AUTHOR(S): Sturgis, B. M.; Baum, A. A.; Trepagnier, J. H.
CORPORATE SOURCE: E. I. du Pont de Nemours & Co., Wilmington, DE
SOURCE: Journal of Industrial and Engineering Chemistry
(Washington, D.C.) (1947), 39, 64-8
CODEN: JIECAD; ISSN: 0095-9014
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

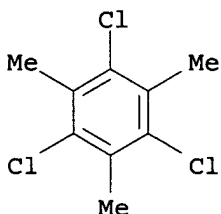
AB In a search for new types of compds. which vulcanize GR-S without S with formation of products with superior resistance to heat, a new class of vulcanizing agents was found comprising halogenated organic compds. which can in turn be divided into 3 groups: (1) chlorinated arylmethyl compds. containing at least 1 substituent Cl atom in the methyl group; (2) halogenated aliphatic hydrocarbons containing at least 1 CX₃ group, where X is Cl, Br, or I; (3) aliphatic compds. containing 1 CCl₃ group attached to a strong polar group. The compds. tested include benzyl chloride, 2,4-dichlorobenzyl chloride, 2,4,6-trichlorobenzyl chloride, benzal chloride, 2,6-dichlorobenzal chloride, benzotrichloride, o-chlorobenzotrichloride, 2,4-dichlorobenzotrichloride, 1-trichloromethyl-naphthalene, 1,1,1,3-tetrachloropropane, 1,1,1-trichloropentane, 1,1,1-trichloroheptane, 1,1,1,9-tetrachlorononane, 1,1,1,5-tetrachloropentane, 1,1,1,5-tetrachloro-2-pentene, octachloro-1,3-pentadiene, hexachloroethane, heptachloropropane, pentachloropropane, pentachloroethane, bromoform, iodoform, C tetrabromide, telomer mixture, trichloroacetic acid, Et trichloroacetate, Zn

trichloroacetate, Pb trichloroacetate, N-trichloroacetylurea, Na trichloroacetate, trichloromethanesulfochloride. All these compds. are unique in that they are primary vulcanizing agents for GR-S, yet do not vulcanize natural rubber in the absence of S. Group (1) members are, in general, the most active and they vulcanize GR-S at room temperature without any accessory agent. A large number of halogenated aromatic compds. including hexachlorobenzene, benzene hexachloride, 9,10-dichloroanthracene, 2,4,6-trichloromesitylene, benzotrifluoride, 2,4,6-trichlorobenzotrifluoride, and other analogous F compds. did not vulcanize GR-S. They are highly activated by some metal oxides, particularly PbO; e.g., with the latter vulcanizates with 2.5% of o-chlorobenzotrifluoride having phys. properties close to those of S vulcanizates are obtained. The oxides tested include CeO₂, Cu₂O, CuO, Pb₃O₄, PbO₂, PbO, MgO, MgO₂, MnO₂, TeO₂, ZnO, and ZnO₂. MgCO₃, CaCO₃, and lithopone also are activators. In group (2), F compds. are inactive, and when alone the Cl and Br compds. are inactive in the absence of a metal oxide; in fact, PbO is the only highly effective oxide. The following compds. were inactive or only slightly active: 1,2,3-tribromobutane, 1,2,3,4-tetrabromobutane, 1,2,3-tribromo-2-methylpropane, 1,2,3,4-tetrachlorobutane, 1,2,3,3-tetrachlorobutane, 1,2,2,3-tetrachlorobutane, 2,2,3-tribromobutane, 1-4-dibromo-2-butene, 1,2-dibromo-1-chloroethane, 3,4-dibromohexane, 1,1,2,2-tetrabromoethane, hexachlorobutadiene, n-butyl iodide, 1,1,7-trichloroheptene, 1,3,3,4,5,6-hexachlorohexane, and methyl iodide. S retards the action of aliphatic halogenated compds. With group (3), both ZnO and S are activating agents and are necessary for the best quality of vulcanizates but they are not necessary to obtain vulcanizates of fair quality. PbO, MgO, Pb₃O₄, MoO₃, and ZnO₂ are less effective activators. That compds. of group (3) are primary vulcanizing agents with S present is evidenced by the fact that amines, e.g. tetraethylenepentamine, activate S alone but retard a combination of S and ethyl trichloroacetate. In general, the halogenated organic vulcanizing agents give GR-S vulcanizates which are characterized by particularly good resistance to elevated temps., e.g. aging at 100°. The mechanism of vulcanization by these compds. does not conform perfectly to any current theories of vulcanization by non-S compds., but the mechanism is possibly analogous to that of BzO₂ (cf. Alfrey, Hendricks, Hershey, and Mark, C.A. 39, 5542.4), i.e.: initial decomposition into free radicals; reaction of the free radicals with the polymer, with elimination of an α -methylenic H atom and formation of an odd electron; reaction of the polymer free radical with a polymer mol., probably with 1 of the double-bond electrons, with cross-linking; and continuation of the process, either by a sequence of cross-linking through the double bonds of addnl. chains or by chain transfer, until a termination reaction takes place.

IT 5324-68-5, Mesitylene, 2,4,6-trichloro-
(as vulcanizing agent in Buna-S)

RN 5324-68-5 CAPLUS

CN Benzene, 1,3,5-trichloro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 14:50:37 ON 02 SEP 2005)

L1 FILE 'REGISTRY' ENTERED AT 14:51:48 ON 02 SEP 2005
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L2 FILE 'CAPLUS' ENTERED AT 14:52:02 ON 02 SEP 2005
STRUCTURE UPLOADED
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L3 FILE 'REGISTRY' ENTERED AT 14:52:33 ON 02 SEP 2005
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L4 FILE 'CAPLUS' ENTERED AT 14:52:34 ON 02 SEP 2005
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L5 FILE 'REGISTRY' ENTERED AT 14:52:45 ON 02 SEP 2005
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S L7

L11 FILE 'REGISTRY' ENTERED AT 14:57:01 ON 02 SEP 2005
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L12 FILE 'CAPLUS' ENTERED AT 14:57:02 ON 02 SEP 2005
347 S L11 SSS FULL
L13 277 S L12 AND PY<1997
L14 10 S L13 AND F AND CL

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